Electronic Supplementary Information:
Levelized cost and carbon intensity of solar hydrogen production from water electrolysis using a scalable and intrinsically safe photocatalytic Z-scheme electrochemical raceway system

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Note 1: Particle Manufacturing.

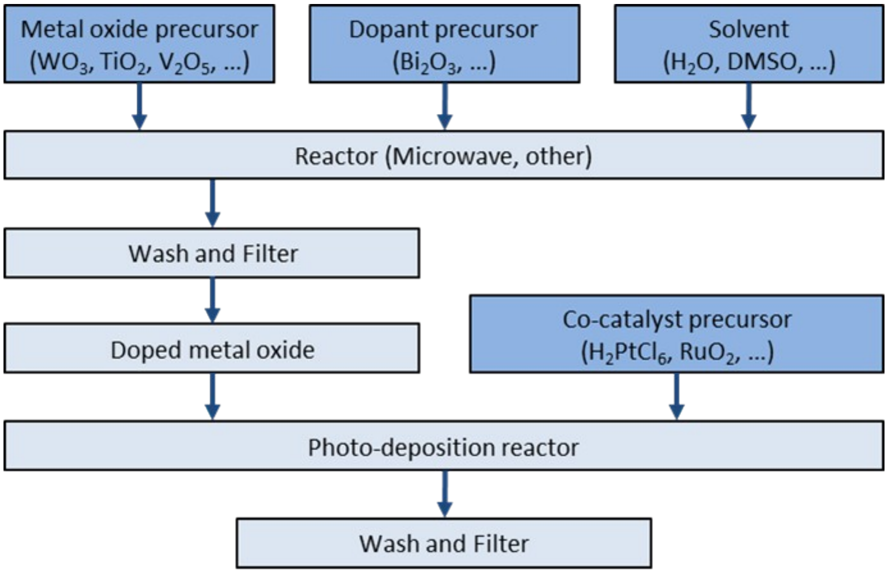

Figure S1. General process flow for catalyst-coated doped metal-oxides

Nano-particle materials development is an active area of investigation, and currently identified catalysts do to meet acceptable levels of conversion efficiency and durability. Consequently, the cost modeling approach is chosen for flexibility and its general applicability to a future nano-particle synthesis process. For this study we selected a solvothermal synthesis pathways since it is scalable for bulk production of doped metal oxides (**Figure S1**). Other pathways (e.g., vapor deposition, pyrolysis, etc.) and coating options may be considered for a future study. While the HER and OER catalysts will be different in an actual system, they are cost modeled here as the same materials for simplicity and since they serve only as placeholders for yet undefined catalyst materials.

Table S1. Range of catalyst particle synthesis costs based on material costs and manufacturing capital costs

Item	Expected Range of Values	Rationale
Annual production	1-500 tonnes/year	Assumed 100 kg per 1 MTD module, 10-500 MTD annual deployment rate, Particle lifetime: 0.5-5 years
Metal oxide salts	\$1-\$100/kg	Range of quotes for bulk (10-1,000 kg) orders of metal oxides
Plant capital cost	\$2M-\$10M	Estimate based on analogous metal organic framework (MOF) analysis scaled for annual material production
Unrecovered solvent costs	\$0-\$25/kg particle	Based on analogous MOF work. Range depends on yield, solvent choice, and recovery
Co-catalyst cost	\$100-\$1,000/kg PC particle	Modeled as 0.2-2 wt% Pt:metal oxide,

		$50k/kgPt
Range of material costs	$100/kg - $1,200/kg PC particle	Materials + Synthesis (approx. first-pass range of particle price)
Range of material prices	**$150/kg - $1,800/kg PC particle**	**50% Manufacturer markup assumed**

Note 2: Balance of Plant (BOP).

A simplified process flow diagram for the PC Type 2 system is shown in **Figure S2**. The H_2 purification subsystem utilizes a deoxidizer to remove O_2 gas impurities from the H_2 gas stream and a Temperature Swing Adsorption (TSA) subsystem to remove vapor water from the H_2 gas stream. Two TSA adsorption beds are used, in alternating cycles, to provide continuous water removal and produce an H_2 product stream with 99.99 mol% H_2 purity. Water removed from the H_2 stream is fed back into the KOH scrubber.

The solar insolation at 35 degrees North varies significantly over the year. The raceway count is sized for the average solar insolation over the year: 1 MTD or 50 MTD on an annual average basis. Consequently, substantially more H_2 is produced in the summer, and substantially less in the winter. Solar insolation in June is 8.39 kWh per m^2 per day which is ~50% more than the average annual insulation. Therefore, the piping and equipment must be sized for this maximum capacity case. Additionally, hourly variation in solar insolation increases beyond even this maximum capacity. For the purposes of this study, it is assumed that sizing the piping and equipment for the highest solar insulation month is sufficient. However, future studies may conclude that further oversizing of piping and equipment is needed for safety or controls purposes i.e., sizing for the highest rate during the highest solar month.

The BOP can be divided into two broad categories: the mechanical BOP and the electrical BOP. The mechanical BOP is composed of four primary elements: process equipment, piping, valves, and instrumentation including temperature, pressure, flow, and level indicators. The electrical BOP consists of 4 primary elements: rectifier, transformer, power substation, and electrical wiring.

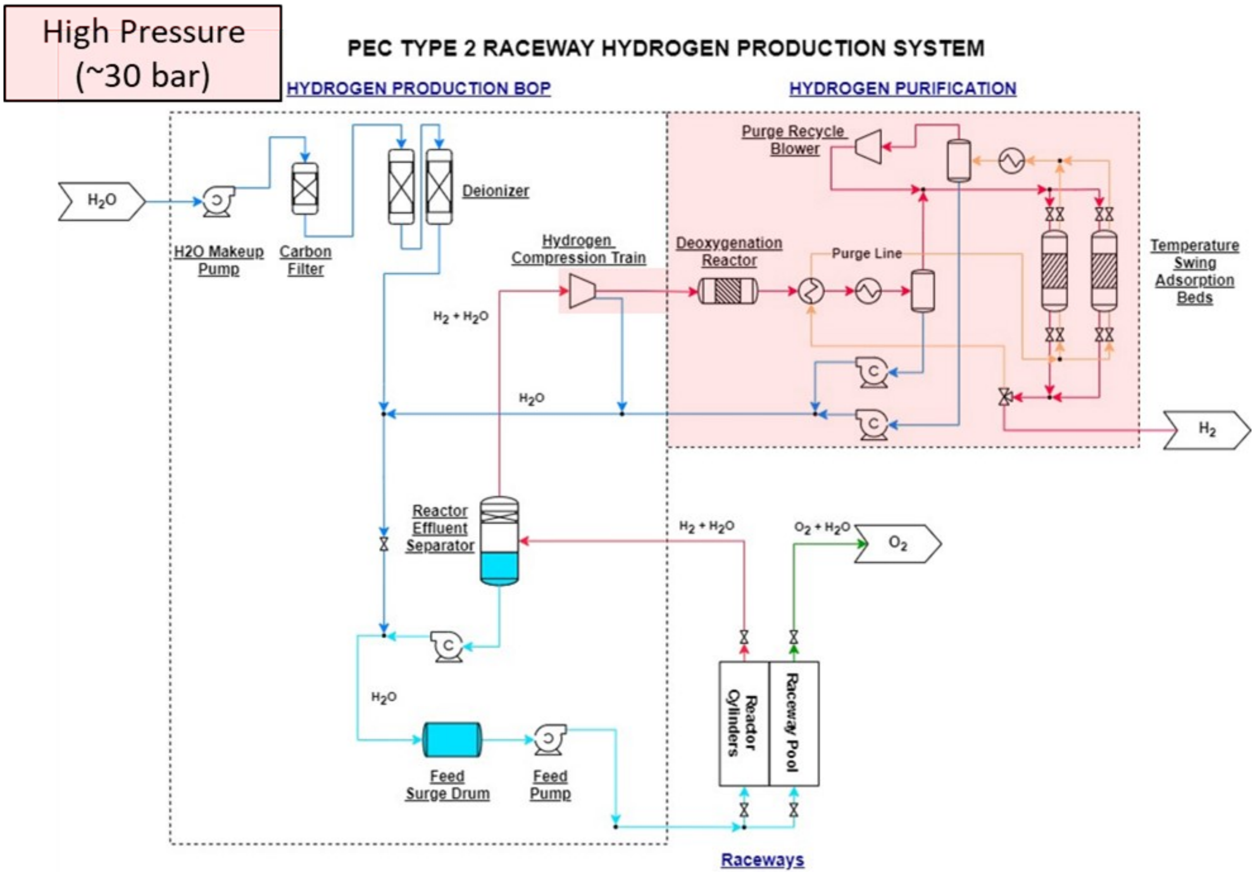

Figure S2. Process flow diagram for PC Type 2 raceway hydrogen production facility

Note 3: Cost Analysis.

Capital Costs.

The cost model used the Aspen Process Economic Analyzer™ (Version 12 (40.0.0.4267)) for preliminary cost estimates of the process equipment and piping. Industry cost curves and historical data were used to empirically estimate costs for valves and instrumentation.[1] The cost model used vendor quotes for the rectifier and an estimate from a 2013 engineering study for the transformer.[*] The electrical wiring was estimated from the 2020 National Electrical Estimator published by Craftsman.[2] The power substation and overhead power lines for external transmission were derived from publicly available price estimates.[†] Where necessary, cost values in this study were adjusted to 2020$ using the Chemical Engineering Plant Cost Index (CEPCI), the standard index used by chemical process industries. All capital costs listed in these tables include vendor markup.

In addition to the direct capital cost of a PC Type 2 plant (including installation of raceways and BOP equipment), the construction of a greenfield electrolysis plant includes two additional cost elements: site preparation and construction overhead (which includes engineering and design fees, up-front permitting costs, and project contingency). The site preparation cost model is based on the system and facility site plans and builds up an overall cost based on estimated labor hour, material cost, and equipment cost data from the Craftsman National Construction Estimator cost data books.[‡] The construction overhead cost model is an empirical exponential scaling model based on publicly available estimates for engineering and design[3, §] (inclusive of procurement and construction activities), and legal and permitting.[**] Project contingency is assumed to be a constant 15% of installed capital cost regardless of project scale.

The balance of plant (BOP) includes all the non-raceway elements described in **Figure S2**, including water inlet and recirculation, hydrogen compression, and hydrogen purification. The complete process including the raceways and the balance of plant constitutes a system. It is assumed that each plant has one system, although future studies may explore multiples systems per plant for the purposes of redundancy or to address limitations in maximum equipment size, particularly for the water purification system, the hydrogen compressor, or the hydrogen purification systems.

A summary of the uninstalled capital costs associated with a raceway is shown in **Table S2**, and visualized in **Figure S3**. The net cost of the uninstalled reactor only components per solar

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[*] $7.5M for 290 MW high temperature steam electrolysis (HTSE) from Krull, P. Roll, J. Varrin, Jr.R.D. "HTSE Plant Cost Model for the INL HTSE Optimization Study," R-6828-00-01, Revision 1, Dominion Engineering, Inc. March 2013.

[†] Cost of the transmission line is set at $390,000/mile. https://www.power-grid.com/td/underground-vs-overhead-power-line-installation-cost-comparison/

[‡] "National Construction Estimator" online cost estimating database by Craftsman Book Company. Free Software download available online at: http://craftsman-book.com

[§] Derived from Fraunhofer estimate of $7.5M for a 100 MW AEL facility.

[**] Permitting costs anchored by a $4.3M cost for a 100 MW facility derived from the most recent DOE H2A ~100 MW solid oxide electrolysis case. https://www.nrel.gov/hydrogen/h2a-production-models.html

incidence area is estimated to be $7.14/m^2, which includes the high density polyethylene (HDPE) film, the polycarbonate filter membrane, the geomembrane, and the port hardware. The HDPE and polycarbonate filter membrane include a 50% manufacturing markup associated with procurement and assembly of reactor cylinders. The total plant direct capital costs (including uninstalled capital costs and installation costs) are shown in **Table S3**, and visualized in **Figure S4**. The biggest cost drivers are the raceways and the control valves associated with managing hydrogen produced from the raceways. These valves will control hydrogen flow rates so that only the rated amount of hydrogen enters the hydrogen compression and purification subsystems. Additional cost optimization of piping and valves may be possible with dynamic simulations to account for hydrogen associated with hourly insolation.

Table S2. Uninstalled Capital Cost for a single Raceway component (2020 US$). Uninstalled reactor only cost includes HDPE (Top Transparent Film), Polycarbonate Filter Membrane (Bottom Ion Bridge), Geomembrane, and Port Hardware.

Raceway Component	Quantity	Unit cost	Overall cost
Reactor			
Reactor Cylinders			
HDPE (Top Transparent Film)	5427 m^2	$ 0.51 / m^2	**$ 2,768**
Polycarbonate Filter Membrane (Bottom Ion Bridge)	4477 m^2	$ 2.62 / m^2	**$ 11,724**
Raceway Reactor Pool			
Geomembrane	3800 m^2	$ 2.92 / m^2	**$ 11,106**
Catalyst Nanoparticles	3.99 kg	$ 450.00 / kg	**$ 1,796**
Reactor Total			**$ 27,393**
Support Hardware			
Port Hardware	300	$ 5.14 / unit	**$ 1,542**
Circulation Pump	1	$ 571.18 / unit	**$ 571**
Bed Wiring Panel	1	$ 166.79 / unit	**$ 167**
Water Level Controllers	1	$ 57.12 / unit	**$ 57**
Pressure Sensors	1	$ 317.58 / unit	**$ 318**
Hydrogen Sensors	1	$ 299.00 / unit	**$ 299**
Instrument Wiring	1	$ 87.96 / unit	**$ 88**
Power Wiring	1	$ 44.55 / unit	**$ 45**
Conduit	1	$ 117.66 / unit	**$ 118**
Support Hardware Total			**$ 3,204**
Total Raceway Cost			**$ 30,597**
Uninstalled Reactor Only Cost	3800 m^2	$ 7.14 / m^2	**$ 27,140**

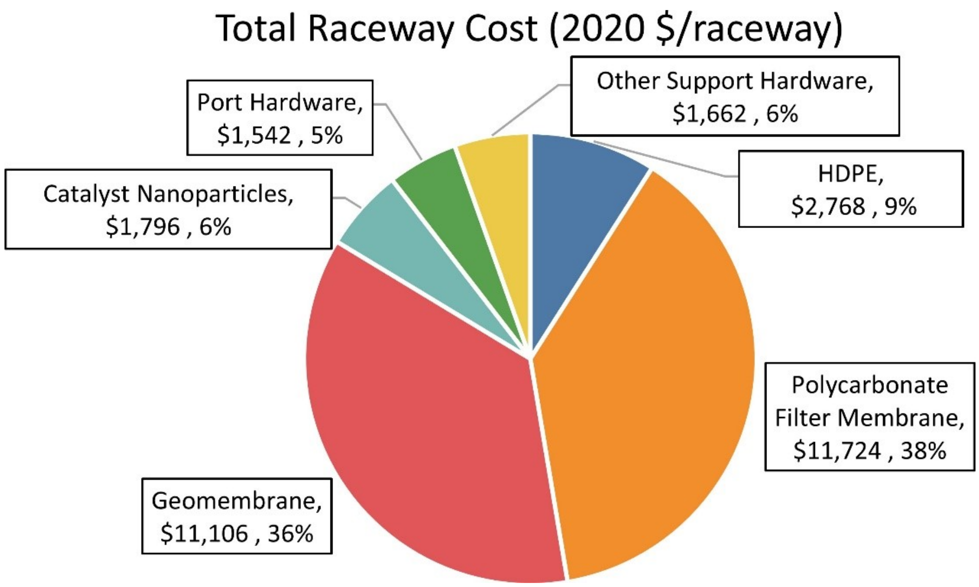


Figure S3. Uninstalled Capital Cost for a single Raceway (2020 $/raceway).

Table S3. Total direct costs for PC Type 2 plant, assuming one system per plant

Plant Capacity	MTD	1	50
Equivalent Electrolyzer Power	MW_AC	2	111
Direct Capital Cost			
Equipment	[2020 $k/system]	$2,026	$16,298
Piping	[2020 $k/system]	$577	$8,374
Purchased Valves	[2020 $k/system]	$280	$7,487
Instrumentation	[2020 $k/system]	$353	$10,682
Wiring	[2020 $k/system]	$182	$2,183
Raceway	[2020 $k/system]	$580	$27,797
Total Direct Capital Costs	**[2020 $k/system]**	**$1,683**	**$28,015**

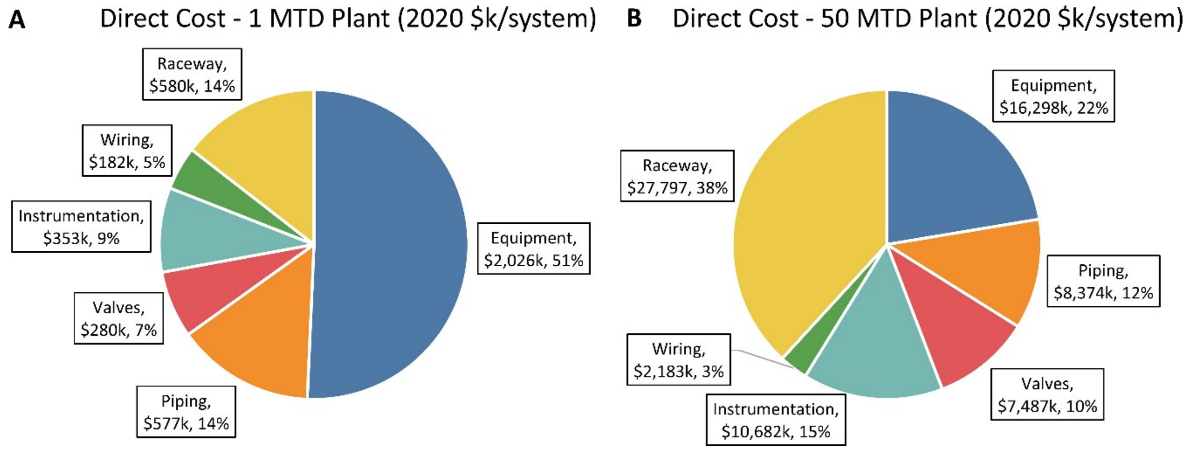


Figure S4. Total direct costs for PC Type 2 plant (2020 $k/system) for A) 1 MTD plant and B) 50 MTD plant

Summarized uninstalled and direct capital costs for a PC Type 2 plant are shown in **Table S4**. Note that all $/kW values are scaled using an estimated equivalent electrolyzer power (1 MTD approximately equal to 2.3 MW and 50 MTD approximately equal to 115 MW). Summarized plant site preparation and construction overhead results are reported for a PC Type 2 plant in **Table S5**. A visualization of the total installed capital cost is shown in **Figure S5.**

Table S4. Uninstalled and direct capital costs for PC Type 2 plant, assuming one system per plant

Plant Capacity	MTD	1	50
Equivalent Electrolyzer Power	MW_AC	2	111
Uninstalled Capital Costs			
Raceway Capital Cost	2020 $k / system	$520	$25,059
Mechanical BOP	2020 $k / system	$1,451	$32,368
Electrical BOP	2020 $k / system	$179	$2,147
Total Uninstalled Capital Costs	**2020 $k / system**	**$2,151**	**$59,574**
Raceway Capital Cost	2020 $ / kW	$226	$225
Mechanical BOP	2020 $ / kW	$629	$291
Electrical BOP	2020 $ / kW	$78	$19
Total Uninstalled Capital Costs	**2020 $ / kW**	**$932**	**$536**
Direct Capital Costs			
Raceway Capital Cost	2020 $k / system	$580	$27,797
Mechanical BOP	2020 $k / system	$3,235	$42,841
Electrical BOP	2020 $k / system	$182	$2,183
Total Direct Capital Costs	**2020 $k / system**	**$3,997**	**$72,822**
Raceway Capital Cost	2020 $ / kW	$251	$250
Mechanical BOP	2020 $ / kW	$1,402	$385
Electrical BOP	2020 $ / kW	$79	$20
Total Direct Capital Costs	**2020 $ / kW**	**$1,732**	**$655**

Table S5. Site preparation and construction overhead for PC Type 2 plant, assuming one system per plant

Plant Capacity	MTD	1	50
Equivalent Electrolyzer Power	MW_AC	2	111
Indirect Capital Costs			
Site Preparation	2020 $k / system	$1,683	$28,015
Engineering and Design	2020 $k / system	$400	$7,282
Up-Front Permitting Costs	2020 $k / system	$600	$4,426
Project Contingency	2020 $k / system	$600	$10,923
Total Indirect Capital Costs	**2020 $k / system**	**$3,282**	**$50,646**
Site Preparation	2020 $ / kW	$729	$252
Engineering and Design	2020 $ / kW	$173	$66
Up-Front Permitting Costs	2020 $ / kW	$260	$40
Project Contingency	2020 $ / kW	$260	$98
Total Indirect Capital Costs	**2020 $ / kW**	**$1,422**	**$456**
Total Indirect Capital Costs	**% of Installed Capital Cost**	**40%**	**31%**

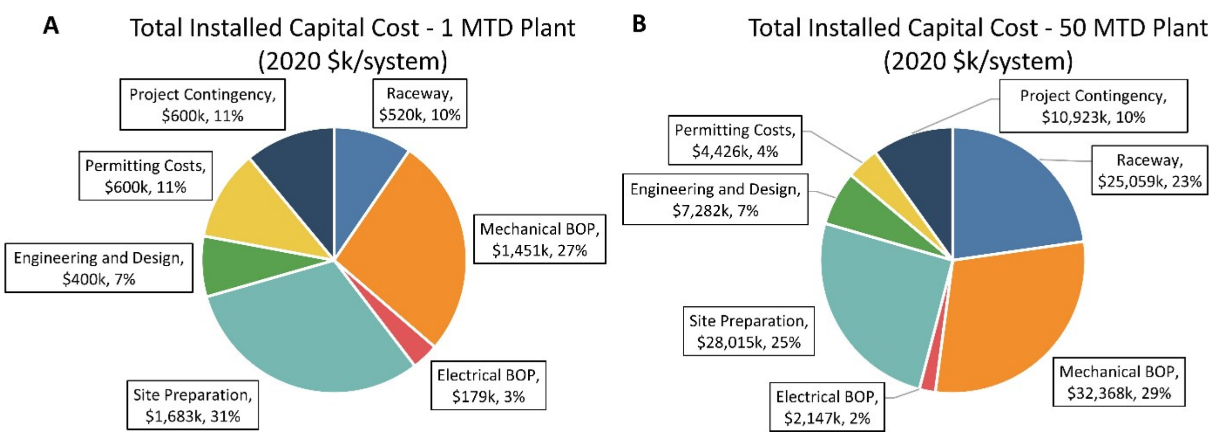


Figure S5. Total installed capital costs for PC Type 2 plant (2020 $k/system) for A) 1 MTD plant and B) 50 MTD plant

Operating Costs.

The operating costs for a PC Type 2 plant are composed of utility costs (electricity), feedstock costs (water), maintenance costs (periodic replacement of raceway reactor components, additional annual costs for all other maintenance activities), and operating labor costs.

Utility cost.

The utilities for a PC Type 2 plant are primarily electricity. Previous LCOH calculations performed using the H2A model used default values to define these utility costs. In particular, the electricity was assumed to follow Annual Energy Outlook (AEO) cost projections for grid-based industrial electricity prices.[4] Based on DOE guidance, a reduced price of 2020 $0.03/kWh was assumed to represent a nominal low-cost electricity price currently possible in specific favorable U.S. markets. Specifically, the baseline electricity price case ($0.03/kWh) corresponds to average wholesale electricity prices currently possible in U.S. markets with plentiful wind.[5] Similar low-cost electricity pricing is possible from solar Power Purchase Agreements (PPA)[6] although these prices are typically limited by renewable energy capacity factors. In this model, 100% availability was assumed to simplify the analysis.

Feedstock cost.

The feedstock for an LA plant is assumed to be water and KOH solution. Water consumption is estimated at 3.78 gallons per kg H_2 inclusive of water converted to H_2 and O_2 and water lost from the system due to purging during water purification, O_2 gas venting, and as an impurity in the H_2 product. No cooling water is assumed in the current process model. The H2A model default water price of ~2020 $0.00237/gal is used. Water loss due to solar energy induced evaporation is not included in this study. The pool is assumed to be covered sufficiently to prevent bulk evaporation. Water inlet from rain is omitted from this study but may further compensate for water inlet costs. Future studies should consider whether water in the pool needs to be continuously purified or whether impurities will cause degradation in solar-to-hydrogen conversion efficiency.

Maintenance cost.

Default H2A model values for the total unplanned replacement capital costs are 0.5% of the total direct depreciable costs per year, and are used in this analysis. In addition to the annual replacement costs, the cost model assumes the reactor cylinders must be replaced every 5 years and the catalyst nanoparticles must be refurbished or replaced every year.

Labor cost.

Labor cost includes charges for plant operation, maintenance, and management. In general, the labor model assumes that labor increases with the number of raceways and major process equipment components, and consequently increases with plant size (due to increasing number of raceways). The number of plant workers per shift is projected by an empirical labor model based on data from five major chemical companies.[7] This corresponds to the staffing used within a conventional chemical plant as opposed to an autonomous or semi-autonomous facility. The model scales with the number of process steps within the plant (excluding process vessels and pumps) and counts each reactor bed as one process step. The associated equation is:

$$N_{operators\ per\ shift} = (6.29 + 0.23N_{process\ steps})^{0.5}$$

The default H2A model assumes 2,080 hours per full-time equivalent (FTE) worker with 8,760 hours per year. While the original reference refers to only operators, this study assumes that this model is inclusive of operation and maintenance workers. Using this definition, the total number of FTE's (including operation and maintenance) is estimated to be 14 FTE's for the 1 MTD case and 69 FTE's for the 50 MTD case. Note that the default H2A model assumes a 20% overhead cost markup on FTE labor, which is assumed to also include administrative and management labor.

H2A model inputs for financial analysis.

An LCOH calculation (using the H2A model) was performed for the 1 MTD and 50 MTD hydrogen plant. The performance and capital cost input parameters and H2A results are shown in **Table S6**.

Table S6. H2A inputs and results for baseline PC Type 2 plant

Plant Capacity	MTD	1	50
Equivalent Electrolyzer Power	MW_AC	2.3	111
Average Production Rate	MTD	1.0	49
Peak Plant Capacity	MTD	1.5	74.2
Land	acres	33	1047
System Performance			
Solar to Hydrogen Efficiency	%	10%	10%
# of Raceways	#	17	819
BOP Electrical Usage (Average)	kWh/kg	3.6	2.5
Capital Cost			
Direct Capital Cost	2020 $k	$3,997	$72,822
Indirect Capital Cost	2020 $k	$3,282	$50,646
Non-Depreciable Capital Cost (Land)	2020 $k	$1,657	$52,337
Total Installed Capital Cost	**2020 $k**	**$8,936**	**$175,805**
Fixed Operating Cost			
Total Plant Staff	H2A FTE	13	63
Total Fixed Operating Cost	2020 $k / year	$1,921	$13,563
H2A Output			
Capital Costs	2020 $ / kg H_2	$2.06	$1.02
Fixed O&M	2020 $ / kg H_2	$5.31	$0.78
Utilities	2020 $ / kg H_2	$0.12	$0.09
Total	**2020 $ / kg H_2**	**$7.51**	**$1.89**

Note 4: Life Cycle Assessment Methods.

The life-cycle assessment was performed from cradle to gate with phases that included site preparation and construction, upstream production and transportation of materials, the operation and maintenance of the facility (including replacement of materials), and the end of life of key material components. Carbon intensity (CI) was the primary concern in this LCA, but seven other midpoint impact categories were assessed including: acidification potential (AP), eutrophication potential (EP), freshwater ecotoxicity potential, human toxicity potential (HTP) – carcinogenic and noncarcinogenic, ozone depletion potential (ODP), and photochemical oxidation potential. CI emission factors for the inputs explicitly modeled in this study and the life-cycle stages depicted in **Figure S6** are listed in **Table S7**. Material quantities are shown in **Table 1** of the main work.

Ecoinvent is a robust, proprietary database that presents more standardized EFs than literature assessments due to consistent system boundaries and assumptions. It also provides access to less popular impact categories that may often be overlooked. However, certain parameters such as electricity and water production are largely subject to regional constraints as exist in this study and therefore literature provides more specific values. As a result, literature values were used for base case CI, while Ecoinvent was used for a global perspective and complete analysis of the remaining impact categories. The complete LCA results are shown in **Figures 4** and **S7**, and the CI sensitivity analysis (**Figure S8**) utilizes EFs from both Ecoinvent and literature to show the impact of changes to specific parameters.

Table S7. Greenhouse gas emission factors for life cycle assessment from literature, presented in units of global warming potential, or carbon dioxide equivalents, per kg material.

Parameter	Unit	Value	Reference
Raceway Materials			
High density polyethylene (HDPE)	kg CO_2eq/kg	1.8	(8) Nicholson et al.
Polycarbonate membrane	kg CO_2eq/kg	8	(8) Nicholson et al.
Geomembrane	kg CO_2eq/kg	1.8	(8) Nicholson et al.
Fe_2O_3 nanoparticles	kg CO_2eq/kg	4	(9) Rahman et al.
TiO_2 nanoparticles	kg CO_2eq/kg	99.3	(10) Wu et al.
Platinum	kg CO_2eq/kg	12,500	(11) Nuss et al.
Piping System			
Polyvinylchloride (PVC) piping	kg CO_2eq/kg	2.45	(12) Wernet et al.
Stainless steel	kg CO_2eq/kg	1.7	Forza Steel
Site Preparation and Construction			
Concrete	kg CO_2eq/m^3	288.1	(13) NRMCA
Reinforcing steel	kg CO_2eq/kg	0.86	(14) Steel Dynamics
Asphalt	kg CO_2eq/kg	0.056	(15) National Asphalt Pavement Association
Truck Transportation	kg CO_2eq/kg-km	0.179	(16) Nahlik et al.
Operation			
Electricity input	g CO_2eq/kWh	218	(17) EGRID EPA
Water (deionized production)	g CO_2eq/kg	0.488	(12) Wernet et al.

Mass and energy flows over the 40-year lifespan of the facility are converted into levelized GHG equivalents using the values in **Table S7** and Equation 1.

$$\frac{\sum U_i \times EF_i \times R_i}{P_{H2} \times 365 \times l}$$

Equation 1

where U_i is the amount of material *i* required in one year, EF_i is the emission factor of material *i,* and R_i is the number of times material *i* is added to the system throughout the analysis period. P_{H2} is the daily rated capacity, and *l* is the plant lifespan.

The energy flows are also incorporated into the calculation for energy return on energy invested (EROEI) which is shown in Equation 2. The EROEI is a unitless ratio showing how much energy is obtained from the system relative to the energy invested in it via materials and energy consumption. Related to the EROEI is the energy payback time (EPBT) which shows how long a system must run in order for it to recover the energy invested over the system lifetime. This is calculated according to Equation 3.

In the analysis for the 1 TPD photocatalytic hydrogen production system, embodied energy was assigned for each life-cycle process input, distinguishing single-use and recurring materials. The embodied energy was obtained from the Ecoinvent database and maintains consistency with the life-cycle emission factors. The embodied energy is allocated to the year where the specific input is deployed. All components are input to the system in year zero for system construction. The construction energy input is –17.8 million kWh. This is the major deficit of the facility that H_2 production needs to overcome. Starting in year 1 of operation there is a nominal embedded energy cost of 5.17 kWh per kg H_2 produced due to consumed water and electricity in addition to nanoparticle replacement. These materials, in addition to raceway plastics and disposal transportation are recurring costs. When hydrogen production begins in year 1, so does the energy payback due to hydrogen having an energy density of 33.3 kWh/kg.

$$\mathrm{EROEI} = \frac{\sum_{t} \mathrm{E_{H2}}}{\sum_{t}\sum_{i} \mathrm{E_{i,t}}}$$

Equation 2

$$\mathrm{EPBT} = \frac{\sum_{t}\sum_{i} \mathrm{E_{i,t}}}{\mathrm{E_{H2}}}$$

Equation 3

E_{H2} is the annual energy output of H_2 (in kWh), and $E_{i,t}$ is the embodied energy (in kWh) of material *i* in year *t*. t in this instance is 41 years to include the 40 years of facility operation and year 0 for construction.

In the case of both TiO_2 and Fe_2O_3, studies estimating manufacturing impact factors from lab-scale data vary from 48.4 to 2.62×10^3 and from 4.00 to 1.40×10^3 respectively, based on the synthesis method.[9,10] Here, we assume solvothermal synthesis for TiO_2 aligning with the production method used in the TEA, and hydrothermal production for Fe_2O_3 where solvothermal was not available. For consistency in comparing the base cases to the scenarios modeled with Ecoinvent which were limited to iron pellet production, the Fe_2O_3 input mass (shown in **Table 1**) is modeled as the Fe mass fraction (70%) of the catalyst amount. Emissions from platinum manufacturing are estimated from a cradle-to-gate analysis, covering the mining to refining of platinum, but not its subsequent treatment to prepare nanoparticles.[11]

Emissions associated with site preparation and construction are simplified to assess only the core materials used. This results in the inclusion of asphalt for pavement, and reinforcing steel and concrete for the building foundation.[13–15]

Transportation is a key source of emissions both in setting up the plant site, and in disposing of materials at the end of the operational period. We assume physical materials disposed of during maintenance and at the facility end of life are sent to a landfill. No landfill GHG emissions are associated with the nanoparticles or plastics so all emissions can be attributed to transportation. With the plant location in CA, we assume plant components are transported via class 8 heavy duty, diesel-powered trucks operating as estimated by CA-GREET.[16] With no specific source of material production and plant operation we approximate the distance traveled by diesel truck for the installation trip and landfill disposal trip each as 150 km per comparable studies.[18] For consistency within the study we include the transport of construction materials to the site and disposal in scope due to emission factors of construction materials being only cradle to gate.

We use an average emission factor for the electricity grid mix in California.[17] This represents a relatively lower impact than the broader US average, but electricity mix is very localized and can be further refined. The use of 100% solar PV in the sensitivity analysis shows the most optimistic electricity performance.

Deionized water is considered necessary for commercial water electrolysis processes, but there is little data on the energy consumption or greenhouse gas emissions of deionized water production in literature. We therefore use the Ecoinvent value in all scenarios of this study and neglect upstream emissions under the assumption that the deionization treatment is the most intensive source of emissions in the water process.[12,19]

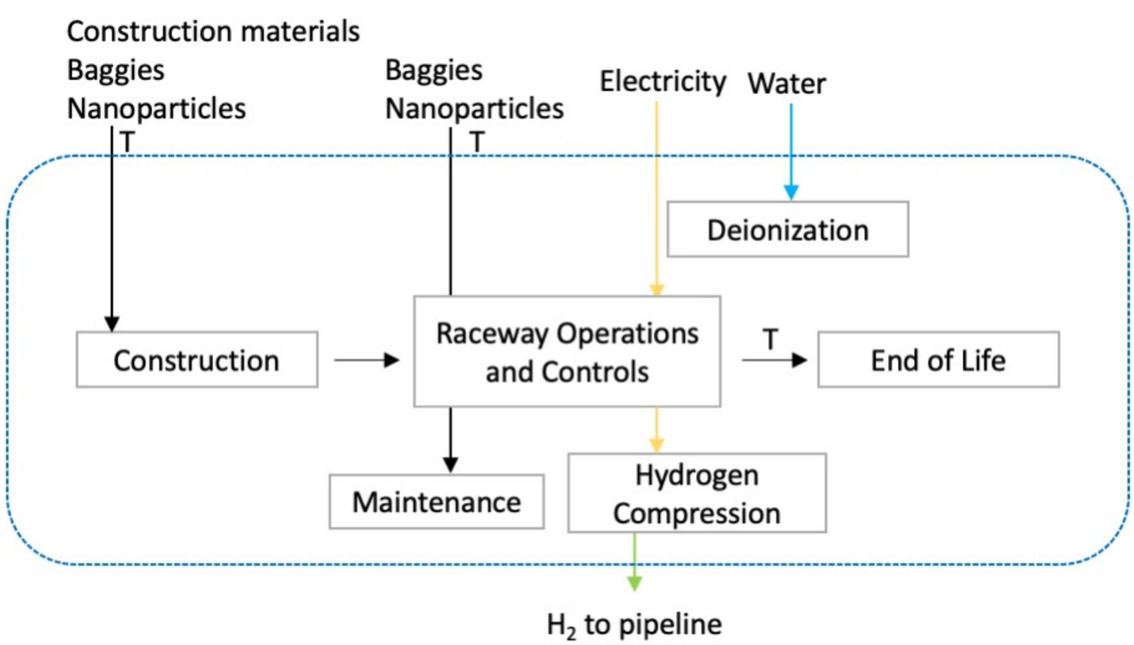


Figure S6. LCA system boundary depicting key processes that were modeled in this study. T: transportation.

Note 5: Life Cycle Assessment Results.

Freshwater ecotoxicity, which refers to the emission of materials toxic to aquatic species in freshwater bodies, is the most concerning result in the LCA, with 110 and 79 cumulative toxicity units (CTUs) per kg H_2 for the 1 and 50 MTD scales respectively. CTU refers to the amount that would a produce a 50% increase in potentially adverse effects. This same metric applies to HTP, which breaks down into carcinogenic toxicity and noncarcinogenic toxicity. HTP-carcinogenic shows low values of 1.67×10^{-6} and 8.46×10^{-7} CTUh for 1 MTD and 50 MTD respectively. Despite being very small values, there is a major difference in these results due to the largest contributing parameter being asphalt. Asphalt does not scale linearly with production capacity and therefore shows a lower levelized impact in the 50 MTD facility. This differs from both freshwater ecotoxicity and HTP-noncarcinogenic which have HDPE, platinum, and electricity as the main contributors. Freshwater ecotoxicity and HTP-noncarcinogenic also show more consistency between the facility scales as HDPE and catalyst materials in particular do scale linearly with production capacity.

Photochemical oxidation potential, which evaluates the potential of emissions to produce smog relative to ozone, has a moderate value of approximately 0.12 kg O_3eq. As with the majority of other impact areas, this is due largely to electricity, and to the platinum and HDPE used in the raceway. Acidification potential (AP) refers to the emission or depositing of acidified materials such as SO_2 or NO_x in the surrounding environment, while eutrophication potential (EP) is the emission of excess nutrients such as phosphorus or nitrogen compounds (represented here as nitrogen equivalents). The disparity between 1 and 50 MTD scales comes from the reduced consumption of construction materials and electricity per kg H_2 at large scales. Lastly, ODP is the category used to assess a process or material's impact on depleting atmospheric ozone. Emissions are modeled in CFC-11 equivalents due to their robust impact on atmospheric ozone. There is negligible impact of H_2 production via PC pathway on atmospheric ozone, which is similar to other H_2 electrolysis studies. The AP assessed here is lower than most other electrolysis production technologies, but evaluation of other impact categories presented here relative to existing technology is challenging because studies present different selections of midpoint categories with different basis units and are therefore not readily comparable.[20–22]

Table S8: LCA results per kg H_2 for all impact categories for both 1 MTD and 50 MTD

Impact Category	1 MTD	50 MTD
Acidification Potential (kg SO_2eq)	9.15×10^{-3}	8.08×10^{-3}
Eutrophication Potential (kg Neq)	1.88×10^{-2}	1.57×10^{-2}
Freshwater Ecotoxicity Potential (CTU)	110	79.0
Carbon Intensity (kg CO_2eq)	1.41	1.15
Human Toxicity Potential Carcinogenic (CTUh)	1.67×10^{-6}	8.46×10^{-7}
Human Toxicity Potential Noncarcinogenic (CTUh)	1.56×10^{-6}	1.37×10^{-6}
Ozone Depletion Potential (kg CFC-11eq)	4.41×10^{-8}	3.93×10^{-8}
Photochemical Oxidation Potential (kg O_3eq)	0.130	0.114

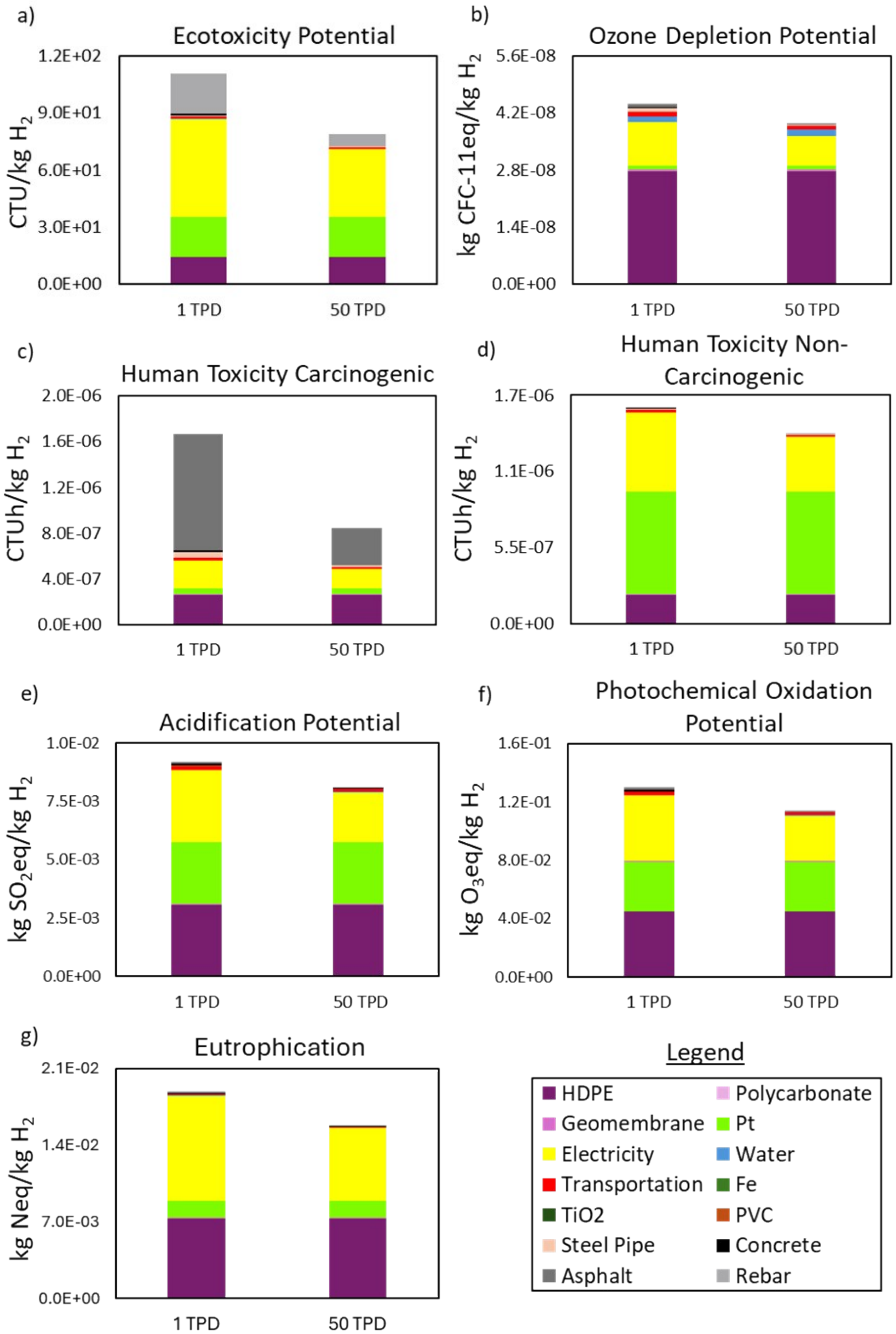
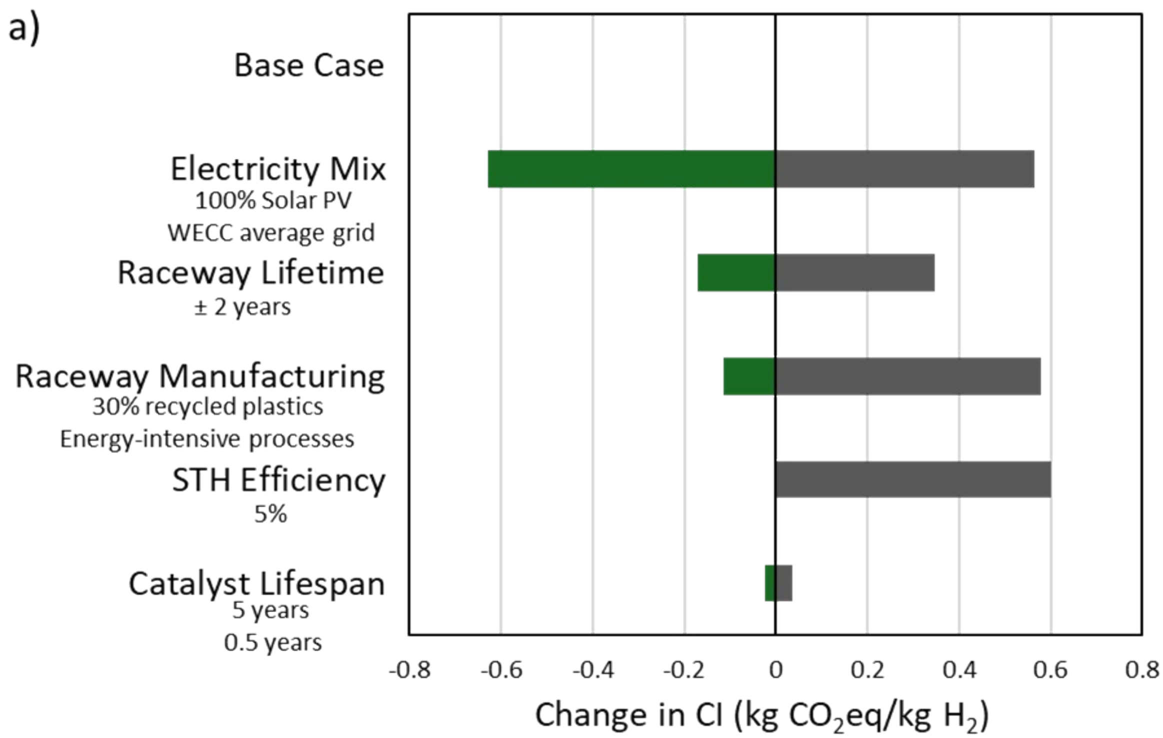


Figure S7: Additional impact categories assessed beyond carbon intensity to evaluate the full impacts of the PC facility design per kg H_2 produced.

A sensitivity analysis was performed to evaluate the impacts of key parameters on the levelized carbon intensity for both production scales. Given the significance of HDPE, platinum, and electricity in the carbon intensity shown in **Figure 4**, these parameters are the focus of the sensitivity analysis. For electricity use, alternative emission factors are available based on the generation source. A range of 100% solar PV as a low emission source, to the Western Electricity Coordinating Council average grid mix as a higher EF is used. Raceway and catalyst lifespans are included in this analysis due to their nature as consumable materials with untested performance. There is variability in how long these materials may last under these operating conditions. Nanoparticle catalysts are assumed to have a one-year lifespan, and in **Figure S8** we show that the levelized emissions can be reduced if the catalysts are able to support up to 5 years of operation before being replaced. Alternatively, there is potential for catalysts to degrade more quickly as well so 0.5 years is assumed as the worst-case operation. The base case assumes that the raceway cylinders have a lifespan of 5 years. To generate a range in which we can sufficiently assess the potential impact of cylinder replacement we use 3- and 7-year lifespans as boundaries. To further assess the impact of raceways, we also include changes in manufacturing assumptions. Optimistic performance assumes that recycled plastics make up 30% of the raceway, while more conservative performance assumes an energy-intensive extrusion process. Additionally, an assessment of lower STH efficiency is included at 5% due to more conservative photocatalytic system performance and to both raceway and catalyst material consumption shifting significantly to maintain the target H_2 output.

In **Figure S8** it is evident that the raceway materials have the greatest impact on the carbon emissions of the production facility due both to the manufacturing processes and raceway lifetime. The large quantity of plastic required in the raceway construction results in a major contribution to the overall GHG emissions. With replacements every 3 years, an additional 3.04 million kg of material is needed (for 1 MTD) thus increasing production and leading to more emissions embodied in the material, and subsequently in transportation. Conversely, extending the lifetime of raceways lowers the plastic consumption and therefore lowers the associated material emissions. The raceway lifespan analysis shows an interesting disparity given the range is $\pm$ 2 years from the base case: The change in CI from a 3-year lifespan is nearly double the change from a 7-year lifespan. This significant difference is due to the assumption in the 3-year replacement scenario, the raceways are replaced at in the 39th year of operation before being decommissioned with the plant in year 40. This results in the allocation of emissions from the replacement to only one year of hydrogen production instead of 3 years, thus increasing the levelized impact. Emissions associated with the plastic used in the raceway are only exacerbated by producing materials using carbon-intensive power sources (Ecoinvent EFs for raceway materials are greater than base case) or additionally by using more energy-intensive manufacturing processes such as plastic extrusion. The combination of carbon-intensive power sources and energy-intensive manufacturing can increase the levelized emissions for both 1 and 50 MTD scales by as much as 0.58 kg CO_2eq. Conversely, HDPE is a readily recyclable material that may lower emissions if used. We thus include an optimistic assessment of the raceway with recycled HDPE comprising 30% of the material. The value of 30% was selected by choosing to assess this scenario with a semi-closed process with the understanding that 30% of HDPE is effectively recycled into new product.[23]

The change of CI due to lower STH efficiency is similar to that of increasing raceway manufacturing CI. This is expected as one of the main parameters being influenced by STH is the number of raceways needed to maintain H_2 output. The choice of electricity generation is secondary to the plastic use but is not negligible. Using 100% solar PV electricity (neglecting storage concerns) for BOP power significantly lowers the carbon intensity by as much as 0.63 kg CO_2eq/kg H_2 for 1 MTD, or by 0.44 kg CO_2e/kg H_2 for 50 MTD. Using a more carbon-intensive power source such as the WECC average mix increases the emissions by 0.56 kg CO_2eq and 0.39 kg CO_2eq for the 1 MTD and 50 MTD scenarios respectively. Lastly, the catalyst lifespan has a nominal effect on emissions overall. Platinum has the largest overall EF in this study but is used in very small amounts. As a result, extending the life of nanoparticle lifespan reduces consumption of platinum (and conversely decreasing lifespan increases consumption), but with so little being used, the change to overall CI is minimal. It is worth noting that changing the amount of material consumed due to lifespan or STH efficiency also affects emissions associated with travel, so the benefits (or costs) associated with the chosen parameter propagate.



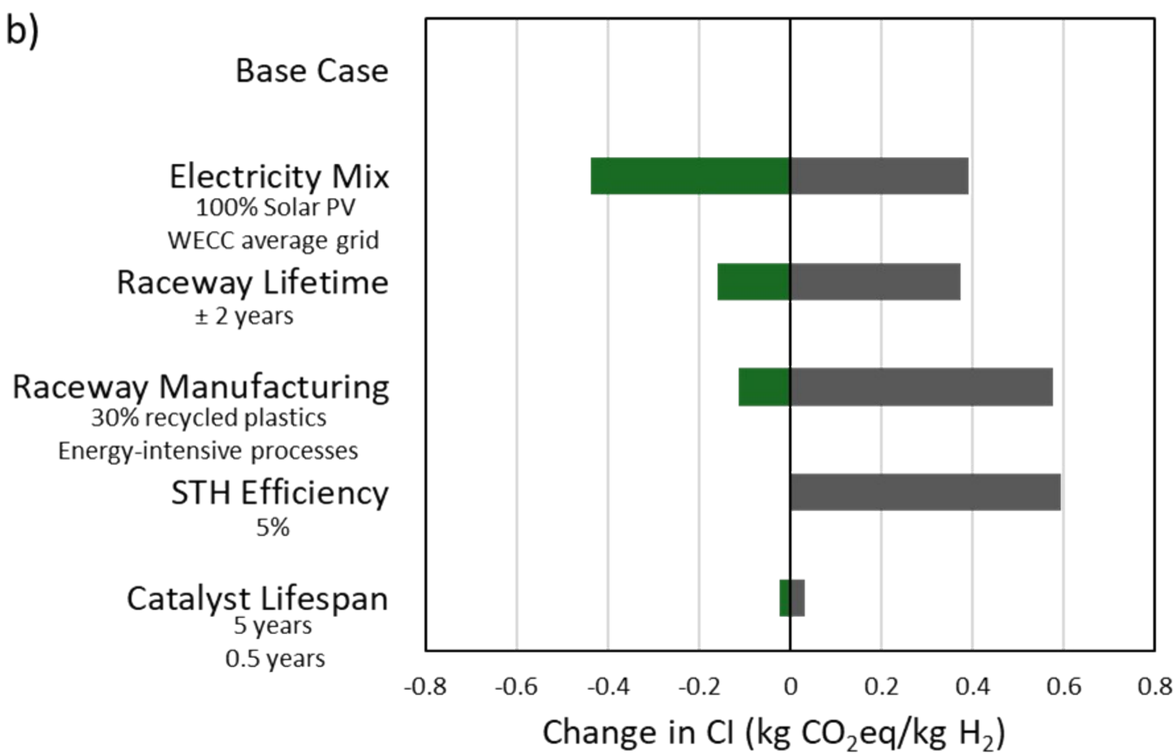


Figure S8. Sensitivity analysis comparing net change in total levelized carbon intensity resulting from changes in STH efficiency, lifespan and manufacturing processes of raceway reactor materials, lifespan of nanoparticle catalysts, and choice of electricity mix for 1 MTD (a) and 50 MTD (b). The base case is the vertical bar intersecting the x-axis at 0.

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